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Extended Abstract
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Chemistry congress: 2019 Cross-sections, transport coefficients and dissociation rate constants of rare gas dimer ions in collision with their parent gas for cold plasma modeling - Benhenni Malika

Benhenni Malika
University of Ostrava, Czech Republic

Transport coefficients and dissociation rate constants of positive rare gas ions are needed input data in chemical electro-hydrodynamic plasma models for a better understanding and optimization of plasma reactors used in applications such as biomedicine or spacecraft. A dynamical hybrid method has been used to calculate momentum transfer for the non-dissociative ion scattering and collision induced dissociation. The hybrid method uses a classical formalism for nuclei and quantum treatment for electrons where the electronic Hamiltonian is calculated via a diatomics-in-molecules (DIM) semiempirical model. Effects of dimer rare gas ion rovibronic excitations are also included in the hybrid dynamical method to improve the agreement between calculated and experimental dimer ion mobility. Moreover, for comparison, momentum-transfer cross-sections have also been derived from an inverse method (based on JWKB approximation and an empirical potential) which fits experimental data available on a limited reduced field range and extends it to a wider range. These collision cross-sections are then used in an optimized Monte Carlo code that simulates the ion trajectory to calculate transport coefficients (mobility and diffusion) and dissociation rate constant of He2+, Ne2+, Ar2+, Kr2+ and Xe2+ dimer ions in collision with their parent gas over a wide range of reduced field.

A quantum formalism and classical treatment are used for electrons and nuclei, respectively, during a hybrid method so as to review the dynamics of electronically ground-state ionic xenon dimer, Xe2+, in its parent gas. A semiempirical Diatomics In Molecules approach has been wont to model the effective electronic Hamiltonian with different sets of input diatomic potentials (ionic and neutral). Non-reactive scattering and collision induced dissociation cross-sections have first been calculated then injected during a Monte Carlo code for the simulations of the transport coefficients and dissociation rate constant calculated at ambient temperature and air pressure .

The collision conditions have a crucial effect on the relative abundances. Energy- and pressure-resolved curves show that the ions formed by a collisionally activated reaction (CAR) process, i.e. [M □ Cl + O]− and [C6H4-n,O2Cln]−•, are favoured by a high of oxygen (3-6 mTorr) (1 Torr = 133.3 Pa) and a coffee collision energy (0.1-7 eV), whereas the ions formed by a collisionally activated dissociation (CAD) process, i.e. [M HCl]−• and Cl−, are favoured by high and high energy. By choosing a comparatively low collision energy (5 eV) and high (4 mTorr), the CAR and CAD ions are often clearly detected. The presence of this intrinsic field results in highly nonlinear behavior; and actually , the dominance of long-range electromagnetic interactions over the short-range interatomic or intermolecular forces is usually cited because the defining characteristic of the plasma state. so as to construct a mathematically rigorous model for the plasma which is additionally accessible to analysis, hypotheses must be imposed which control these nonlinearities.

Plasma modeling refers to solving equations of motion that describe the state of a plasma. it's generally including Maxwell's equations for electromagnetic fields or Poisson's equation for electrostatic fields. There are several main sorts of plasma models: single particle, kinetic, fluid, hybrid kinetic/fluid, gyrokinetic and as system of the many particles. to scale back the complexities within the kinetic description, the fluid model describes the plasma supported macroscopic quantities (velocity moments of the distribution like density, mean velocity, and mean energy). The equations for macroscopic quantities, called fluid equations, are obtained by taking velocity moments of the Boltzmann equation or the Vlasov equation. The fluid equations aren't closed without the determination of transport coefficients like mobility, diffusion coefficient, averaged collision frequencies, and so on. to work out the transport coefficients, the speed distribution function must be assumed/chosen. But this assumption can cause a failure of capturing some physics

In the gyrokinetic model, which is acceptable to systems with a robust background magnetic flux , the kinetic equations are averaged over the fast circular motion of the gyroradius. This model has been used extensively for simulation of tokamak plasma instabilities (for example, the GYRO and Gyrokinetic ElectroMagnetic codes), and more recently in astrophysical applications. Quantum methods aren't yet quite common in plasma modeling. they will be wont to solve unique modeling problems; like situations where other methods don't apply. They involve the appliance of quantum theory to plasma. In these cases, the electrical and magnetic fields made by particles are modeled sort of a field; an internet of forces. Particles that move, or are faraway from the population push and pull on this web of forces, this field. The mathematical treatment for this involves Lagrangian mathematics.

E-mail: benhenni@laplace.univ-tlse.fr